

2.6 Propagators and Feynman path integrals

47

REF:

Gottfried and Yan
ch. 2.6, 2.7

(1) propagators

* Remark

These particular formulations of QM are used typically for the "many"-particle QM, but we just consider a single-particle case only, for the simplicity.

- Time evolution of a state $|\alpha\rangle$

$$\Rightarrow |\alpha, t_0; t\rangle = U(t, t_0) |\alpha, t_0\rangle$$

This is what we know.

and the Schrödinger eq.

$$\Rightarrow i\hbar \frac{\partial}{\partial t} U(t, t_0) = H(t) U(t, t_0) \quad \leftarrow \text{we also know this.}$$

by multiplying $\langle \vec{x}_1 | \cdot$, $t \rightarrow t_1$

$$\psi_\alpha(\vec{x}_1, t_1) = \int d^3x_0 \langle \vec{x}_1 | U(t_1, t_0) | \vec{x}_0 \rangle \psi_\alpha(\vec{x}_0, t_0)$$

: It moves the state both into

the future and the past.

$$\psi_\alpha(\vec{x}, t) = \langle \vec{x} | \alpha, t \rangle$$

↓

Choose the future:

$$\psi_\alpha(\vec{x}_1, t_1) = \int d^3x_0 K(\vec{x}_1, t_1, \vec{x}_0, t_0) \psi_\alpha(\vec{x}_0, t_0)$$

where

$$K(\vec{x}_1, t_1, \vec{x}_0, t_0) = \langle \vec{x}_1 | U(t_1, t_0) | \vec{x}_0 \rangle$$

$$\Theta(t_1 - t_0)$$

⇒ It's a causal theory.

future!

: time-evolution (unitary) of a wave function

is deterministic.

→ Limiting behavior at $t_1 \rightarrow t_0$ d=3 in 3D. 48

$$\lim_{t_1 \rightarrow t_0} K(\vec{x}_1, t_1; \vec{x}_0, t_0) = \delta^d(\vec{x}_1 - \vec{x}_0) \quad \parallel \quad \lim_{t_1 \rightarrow t_0} U(t_1, t_0) \rightarrow 1$$

→ Interpretation as a transition probability (amplitude)

$$K(\vec{x}_1, t_1; \vec{x}_0, t_0) = \langle \vec{x}_1, t_1 | \vec{x}_0, t_0 \rangle \quad \parallel \quad |\vec{x}_0, t_0\rangle = |\vec{x}_0\rangle$$

Composition property:

$$K(\vec{x}_2, t_2; \vec{x}_0, t_0) = \int d^3x_1 K(\vec{x}_2, t_2; \vec{x}_1, t_1) K(\vec{x}_1, t_1; \vec{x}_0, t_0) \quad (t_2 > t_1 > t_0)$$

finding the system at (\vec{x}_1, t_1) ,
(particle)

given that it was originally at (\vec{x}_0, t_0) .

→ How can we compute K ?

① If we know all E 's and ψ 's → trivial. (see below)

② One can get it directly from H :

$$\left[i\hbar \frac{\partial}{\partial t} - H(\vec{x}, t) \right] K(\vec{x}, t; \vec{x}_0, t_0) = i\hbar \delta(t - t_0) \delta^d(\vec{x} - \vec{x}_0)$$

... inhomogeneous part of the Schrödinger eq.

verification

$$i\hbar \frac{\partial}{\partial t} K = i\hbar \langle \vec{x} | \frac{\partial}{\partial t} U(t, t_0) | \vec{x}_0 \rangle \Theta(t - t_0)$$

$$+ i\hbar \langle \vec{x} | U(t, t_0) | \vec{x}_0 \rangle \delta(t - t_0)$$

$$= \langle \vec{x} | H U(t, t_0) | \vec{x}_0 \rangle \Theta(t - t_0)$$

$$+ i\hbar \langle \vec{x} | \vec{x}_0 \rangle \delta(t - t_0)$$

$$= H(\vec{x}, t) K(\vec{x}, t; \vec{x}_0, t_0)$$

$$+ i\hbar \delta(t - t_0) \delta^d(\vec{x} - \vec{x}_0)$$

NOTE: "local" potential.

$$H(\vec{x}, t) = \langle \vec{x} | H | \vec{x}' \rangle$$

$$= H(\vec{x}, t) \delta(\vec{x} - \vec{x}')$$

$$\text{ex. } -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x})$$

$$\leftarrow \lim_{t \rightarrow t_0} U(t, t_0) = 1$$

→ dimension of K ?

49

$$[i\hbar \partial_t - H] K = i\hbar \delta(t-t_0) \delta^d(\vec{x}-\vec{x}_0)$$

$\underbrace{\hspace{10em}}_{\text{energy} = [H] T^{-1}} \quad \underbrace{\hspace{10em}}_{L T^{-1}} \quad \underbrace{\hspace{10em}}_{L^{-d}}$

$$\Rightarrow [K] = L^{-d} \quad \star$$

(2) Green's Functions

\star t -indep. $H \Rightarrow U(t, t_0) = \exp \left[-\frac{i}{\hbar} H(t-t_0) \right]$

: time-evolution operator depends only on $t-t_0$!

→ let $t-t_0 \equiv t$.

• propagator $K(\vec{x}_1, \vec{x}_0; t) \equiv \langle \vec{x}_1 | e^{-\frac{i}{\hbar} H t} | \vec{x}_0 \rangle \Theta(t)$

If we know all E_n 's and $\{ |n\rangle \}$,

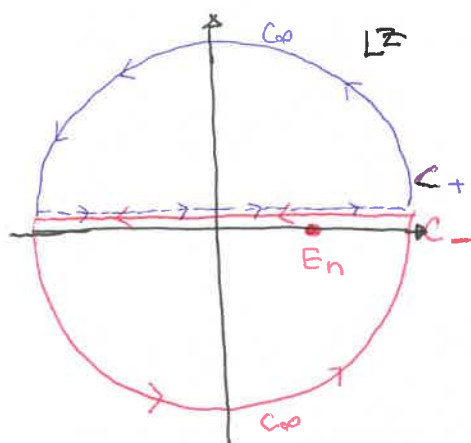
$$K(\vec{x}_1, \vec{x}_0; t) = \Theta(t) \sum_n e^{-\frac{i}{\hbar} E_n t} u_n(\vec{x}_1) u_n^*(\vec{x}_0)$$

⇒ Integral representation

$$K(\vec{x}_1, \vec{x}_0; t) = \frac{i}{2\pi} \int_{-\infty+i\epsilon}^{\infty+i\epsilon} dz e^{-\frac{i}{\hbar} z t} \sum_n \frac{u_n(\vec{x}_1) u_n^*(\vec{x}_0)}{z - E_n}$$

$u_n(x) = \langle x | n \rangle$
: energy
eigenfunction

Check: $\int_{-\infty+i\epsilon}^{\infty+i\epsilon} dz e^{-\frac{i}{\hbar} z t} \frac{1}{z - E_n}$



i) $t > 0$

$$\int_{C_-} = - \int_{-\infty+i\epsilon}^{\infty+i\epsilon} + \int_{C_0} = 2\pi i e^{-\frac{i}{\hbar} E_n t}$$

ii) $t < 0$

$$\int_{C_+} = \int_{-\infty+i\epsilon}^{\infty+i\epsilon} + \int_{C_0} = 0$$

"no pole"

→ Green's function (inverse transformation)

50.

$$\underline{G(\vec{x}_1, \vec{x}_0; E)} = \frac{1}{i\hbar} \int_0^\infty dt e^{i(E+i\epsilon)t/\hbar} K(\vec{x}_1, \vec{x}_0; t)$$

$$= \sum_n \frac{U_n(\vec{x}_1) U_n^*(\vec{x}_0)}{E - E_n + i\epsilon}$$

• How to get it from H :

$$[E - H(\vec{x})] G(\vec{x}, \vec{x}_0; E)$$

$$= \sum_n \frac{[E - H(\vec{x})] U_n(\vec{x}) U_n^*(\vec{x}_0)}{E - E_n + i\epsilon} = \sum_n U_n(\vec{x}) U_n^*(\vec{x}_0)$$

$$= \delta^d(\vec{x} - \vec{x}_0)$$

$$\Rightarrow \boxed{(E - H(\vec{x})) G(\vec{x}, \vec{x}_0; E) = \delta^d(\vec{x} - \vec{x}_0)}$$

... inhomogeneous Schrödinger eq.

with a source term.

(3) Free particle K and G. ... examples in "1D"

• No potential : $H = \frac{1}{2m} \tilde{p}^2$

• free-particle propagator $\sum |p\rangle \langle p|$ $\sum |p'\rangle \langle p'|$

$$K(x, x'; t) = \langle x | e^{-\frac{i}{2m\hbar} \tilde{p}^2 t} | x' \rangle \Theta(t)$$

• H is translation invariant : We can just set $x'=0$

$$\Rightarrow K(x, t) = \Theta(t) \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar} [px - \frac{p^2 t}{2m}]} \parallel \begin{aligned} &\langle x | p \rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} e^{i \frac{px}{\hbar}} \end{aligned}$$

$$K(x, t) = \Theta(t) \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp \left[-\frac{i t}{2m\hbar} \left(p - \frac{m}{t} x \right)^2 + i \frac{m x^2}{2\hbar t} \right] \quad (5)$$

→ just Gaussian integration.

$$= \Theta(t) \sqrt{\frac{m}{2\pi i\hbar t}} \exp \left[i \frac{m x^2}{2\hbar t} \right]$$

Fresnel

... easy to generalize to 3D cases. // This is it.

• free-particle Green's function (3D)

$$(\nabla^2 + k^2) G(\vec{x}, k) = \delta(\vec{x})$$

→ Helmholtz eq. $\parallel k^2 = \frac{2mE}{\hbar^2}$

$$\int_{-\infty}^{\infty} dx e^{-\frac{1}{2}|a|x^2} = \sqrt{\frac{\pi}{|a|}}$$

$$= \sqrt{\frac{\pi}{\pm i|a|}} = \begin{cases} \sqrt{\frac{\pi}{i|a|}} \\ \sqrt{\frac{\pi}{-i|a|}} \end{cases}$$

$$\Rightarrow G_{\text{ret}}(\vec{x}, k) = -\frac{1}{4\pi} \frac{e^{i k r}}{r} \quad \text{outgoing } (E \rightarrow E + i\epsilon)$$

"retarded" (going to the future) \uparrow $t > 0$

c.f., if we set $E \rightarrow E - i\epsilon$ ($t < 0$)

$$G_{\text{adv}}(\vec{x}, k) = -\frac{1}{4\pi} \frac{e^{-i k r}}{r} \quad (\text{incoming})$$

"advanced" (coming back to the past)

(4) Perturbation Theory *

... This is what all these things are about.

$$H = H_0 + V$$

→ Suppose that we know K_0 and G_0 .

• propagator.

for H :

$$[i\hbar \partial_t - H_0] K(x_1 t_1, x_2 t_2)$$

$$= V(x_1 t_1) K(x_1 t_1, x_2 t_2) + i\hbar \delta^4(x_1 - x_2) \delta(t_1 - t_2)$$

for H_0 :

$$[i\hbar \partial_t - H_0] K_0(x_1 t_1, x_2 t_2) = i\hbar \delta^4(x_1 - x_2) \delta(t_1 - t_2)$$

$$\Rightarrow [\hat{H}_0 - H_0] (K(x_1, t_1, x_2, t_2) - K_0(x_1, t_1, x_2, t_2)) \\ = V(x_1, t_1) K(x_1, t_1, x_2, t_2)$$

$$\Rightarrow K(x_1, t_1, x_2, t_2) = K_0(x_1, t_1, x_2, t_2) \\ + \frac{1}{i\hbar} \int dx_3 dt_3 K_0(x_1, t_1, x_3, t_3) V(x_3, t_3) K(x_3, t_3, x_2, t_2)$$

Let $1 \equiv (x_1, t_1)$, $2 \equiv (x_2, t_2)$, $3 \equiv (x_3, t_3)$

$$K(1, 2) = K_0(1, 2) + \frac{1}{i\hbar} \int d3 K_0(1, 3) V(3) K(3, 2)$$

perturbation expansion.

$$\hookrightarrow K(1, 2) = K_0(1, 2) + \frac{1}{i\hbar} \int d3 K_0(1, 3) V(3) \underline{K_0(3, 2)} \\ + \left(\frac{1}{i\hbar}\right)^2 \int d3 d4 K_0(1, 3) V(3) K_0(3, 4) V(4) K_0(4, 2) \\ + \left(\frac{1}{i\hbar}\right)^3 \dots + \left(\frac{1}{i\hbar}\right)^4 \dots$$

• Green's function.

\hookrightarrow Its operator contains the resolvent.

projection op.

$$\underline{\text{def.}} \quad G(z) \equiv \frac{1}{z - H} = \sum_n |n\rangle \frac{1}{z - E_n} \langle n| = \sum_n \frac{P_n}{z - E_n}$$

\downarrow Schrödinger eq.

\hookrightarrow Green's function

$$\underline{G(\vec{x}, \vec{x}'; E) = \langle \vec{x} | G(E + i\epsilon) | \vec{x}' \rangle}$$

\downarrow

$$\underline{(z - H) G(z) = \mathbb{1}}$$

$$(E - H) G(\vec{x}, \vec{x}'; E) = \delta(\vec{x} - \vec{x}')$$

well-defined

as long as z is not on the real axis.

now, $H = \underline{H_0 + V}$ vs $\underline{H_0}$

53

$$\Rightarrow G(z) = \frac{1}{z - H_0 - V} \quad \text{vs} \quad G_0(z) = \frac{1}{z - H_0}$$

By using the identity, $\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A-B}$

$$= \frac{1}{A} + \frac{1}{A-B} B \frac{1}{A}$$

$$\Rightarrow \underline{G = G_0 + G_0 V G} \quad \begin{array}{l} A \equiv z - H_0 \\ B \equiv V \end{array}$$

$$\hookrightarrow G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \dots$$

... Born series "

\Rightarrow Integral equation for the Green's function.

$$G(\vec{r}, \vec{r}') = G_0(\vec{r}, \vec{r}') + \int d\vec{s} G_0(\vec{r}, \vec{s}) V(\vec{s}) G(\vec{s}, \vec{r}')$$

|| E is omitted.

(5) The Feynman Path Integral. "

$= S$ (classical action).

Dirac: $\exp\left[\frac{i}{\hbar} \int_{t_1}^{t_2} dt L_{\text{classical}}\right]$ corresponds to $\langle x_2, t_2 | x_1, t_1 \rangle$.

???

Feynman: $\exp\left[\frac{i}{\hbar} S\right]$ is proportional to $\langle x_2, t_2 | x_1, t_1 \rangle$.

path integral

$$\Rightarrow \langle x_N, t_N | x_1, t_1 \rangle = \int_{x_1}^{x_N} \mathcal{D}[x(t)] e^{\frac{i}{\hbar} S[x(t)]}.$$